

Formation and Relaxation Energies of Electronic Holes in LaMnO_3 Crystal*

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Using the Mott-Littleton approach we evaluate electronic and ionic polarisation energies in the LaMnO_3 lattice associated with localized holes on both cation Mn^{3+} and anion O^{2-} . The full (electronic and ionic) lattice relaxation energy for a localized a hole at the O-site is estimated as 2.4 eV which is appreciably greater than that of 0.8 eV for a hole localized at the Mn-site. We also examine the energies of a number of thermal and optical transitions involving Mn^{4+} , O^- and La^{4+} in the LaMnO_3 lattice. For these calculations we derive a phenomenological value for the second electron affinity of oxygen in LaMnO_3 lattice by matching the optical energies of La^{4+} and O^- hole formation with maxima of binding energies in the experimental photoemission spectra. The calculated thermal energies (one part of the self-trapping energy) predict that the electronic hole is marginally more stable in the Mn^{4+} state of the LaMnO_3 host lattice, but the energy of a hole in the O^- state is only higher by a small amount, 0.75 eV, rather suggesting that both possibilities should be treated seriously.

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